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Effect of boundary conditions on the critical behavior of a finite high-dimensional Ising model

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Finite-size behavior of the $d>4$ Ising model with free boundary conditions is studied by a novel technique of expanding the order parameter in standing-wave modes. Results are reported for the behavior of the susceptibility in various temperature regimes near the bulk critical point. A large "nonscaling" temperature shift is needed to describe the scaling properties.

The critical behavior of the *infinite* Ising model in $d>4$ dimensions is asymptotically mean-field-like and thus, in a sense, trivial. Finite-size behavior, however, poses some interesting theoretical challenges.[1-6] For one thing, hyperscaling is known not to hold for the Ising model above four dimensions, which entails a breakdown of the single-length-scale (correlation length) domination of critical fluctuations on approach to criticality.[2] It is then not obvious, *a priori,* what length (or lengths) should be used to "scale" the system size L in writing finite-size scaling relations.

For systems with *periodic* boundary conditions, the issue has been resolved recently.[2,3,5,6] We will summarize some of the results, which were confirmed by numerical studies,[3,4] later.

In this Rapid Communication we consider the case of *free boundary conditions.* We will concentrate on the susceptibility χ. Hyperscaling and finite-size scaling predict[7] the following power-law divergence for χ at the bulk critical point as a characteristic linear dimension L of the finite system goes to infinity:

$$\chi(L)\propto L^{\gamma/\nu} \quad . \tag{1}$$

The quantities γ and ν are the bulk critical exponents for the susceptibility and correlation length, respectively. This relationship is known to be violated in the case of an Ising model with periodic boundary conditions in more than four dimensions. There one has $\gamma=1$ and $\nu=\frac{1}{2}$, while at the bulk critical point[1-6]

$$\chi(L)\propto L^{d/2} \quad . \tag{2}$$

The above result *cannot hold* for free boundary conditions, because it lies above a strict upper bound[8] established with the use of fluctuation-response relations and Griffiths inequalities: In a finite Ising model with free boundary conditions the susceptibility at the bulk critical point cannot diverge more rapidly than $L^{\gamma/\nu}$ or, in more than four dimensions, than L^2. Because (2) applies to a system with periodic rather than free boundary conditions, one is left with the clear implication that the effects of boundary conditions on the critical behavior of a finite system can be considerable.

The mechanism by which relation (1) and the hyperscaling are violated in the periodic case has been elucidated in Refs. 2 and 3. The critical contribution to the free energy of a finite Ising model has the following form, consistent with the renormalization group, when $d>4$:

$$F^{(s)}=G(tL^2,hL^{(d+2)/2},uL^{4-d}) \quad , \tag{3}$$

where t $[\equiv(T-T_c)/T_c]$ is the reduced bulk temperature (without a size-dependent shift[7]), h is the ordering field, and the quantity u is the leading irrelevant variable. Hyperscaling fails because u is a *dangerous* irrelevant variable;[2,9] it cannot always be set equal to zero. In the case of the zero-field susceptibility,

$$\chi=-V^{-1}(\partial^2F^{(s)}/\partial h^2)_{h=0} \quad ;$$

where $V\equiv L^d$, we have, from (3),

$$\chi\approx L^2X(tL^2,0,uL^{4-d}) \quad . \tag{4}$$

When $t=0$, the function $X(0,0,s_3)$ behaves as $s_3^{-1/2}$. Thus

$$\chi_{t=0}\sim L^2/(uL^{4-d})^{1/2}=u^{-1/2}L^{d/2} \quad , \tag{5}$$

and the result (2) is recovered.

We assess the effects of boundary conditions by calculating the leading contribution to the susceptibility of a finite Ising model in more than four dimensions (subject to free boundary conditions). We find that χ indeed grows as L^2 at the bulk critical point and discuss its dependence on size and temperature when $T\gtrsim T_c$. Calculations on this system when $T\lesssim T_c$ are significantly more difficult than is the case for periodic boundary conditions, in which the leading contributions to χ can be obtained[2,3,5,6] by performing a single integral. A straightforward calculational strategy exists, however, that allows one to treat the case of free boundary conditions.

An important difference between the Ising models with periodic and free boundary conditions is in the modes used in the expansion of the Landau-Ginzburg-Wilson effective Hamiltonian of the systems. One uses complex-exponential plane waves for periodic boundary conditions, while free boundary conditions, which are essentially the same as those for a (coarse-grained) system whose order parameter vanishes at the boundaries, require the use of standing waves. For a d-dimensional rectangular sample located at $0\leqslant x_j\leqslant L_j$ $(j=1,2,\ldots,d)$ the standing waves have the following spatial dependence:

$$\psi_{\mathbf{k}}(\mathbf{x}) = \prod_{j=1}^{d} (2/L_j)^{1/2} \sin(k_j x_j) \ , \tag{6}$$

where

$$k_j = n_j \pi / L_j \ , \tag{7}$$

the n_j's being positive integers. Expanding the order parameter $\sigma(\mathbf{x})$ in these modes, i.e.,

$$\sigma(\mathbf{x}) = \sum_{\mathbf{k}} A_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{x}) \ , \tag{8}$$

we have for the effective Hamiltonian

$$\begin{aligned}\beta H[\sigma(\mathbf{x})] &= \int_V d^d x \, \{\tfrac{1}{2} r[\sigma(\mathbf{x})]^2 + \tfrac{1}{2}|\nabla\sigma(\mathbf{x})|^2 + u[\sigma(\mathbf{x})]^4 - h\sigma(\mathbf{x})\} \\ &= \tfrac{1}{2}\sum_{\mathbf{k}} (r+k^2) A_{\mathbf{k}}^2 - \left(\frac{8}{\pi}\right)^{d/2} h \sum_{\mathbf{k}}{}^{\rm o} A_{\mathbf{k}} \prod_{j=1}^{d} (n_j k_j)^{-1/2} + uV^{-1} \sum_{\mathbf{k},\mathbf{q},\mathbf{p},\mathbf{l}} A_{\mathbf{k}} A_{\mathbf{q}} A_{\mathbf{p}} A_{\mathbf{l}} \prod_{j=1}^{d} \Delta_{k_j q_j p_j l_j} \ ,\end{aligned} \tag{9}$$

where

$$\Delta_{abcd} \equiv \frac{1}{2} \sum_{\alpha=\pm 1} \sum_{\beta=\pm 1} \sum_{\gamma=\pm 1} (-1)^{\alpha+\beta+\gamma} \delta_{a+\alpha b+\beta c+\gamma d} \ . \tag{10}$$

The sum $\sum^{\rm o}$ is only over $\mathbf{k}$'s associated with *odd* values of *all* n_j's. The bulk critical point is at $h=r=0$.

Neglecting for the time being the quartic term in (9), we calculate the zero-field susceptibility in the Gaussian approximation,

$$\begin{aligned}\chi &\equiv V^{-1}(\partial^2/\partial h^2)\ln\left(\int D\sigma \exp\{-\beta H[\sigma(\mathbf{x})]\}\right) = 8^d \sum_{\mathbf{k}}{}^{\rm o} (r+k^2)^{-1} \prod_{j=1}^{d} (k_j L_j)^{-2} \\ &= \left(\frac{8}{\pi^2}\right)^d \sum_{\mathbf{n}}{}^{\rm o} \frac{1}{n_1^2 n_2^2 \cdots n_d^2} \frac{1}{r + (\pi/L_1)^2 n_1^2 + \cdots + (\pi/L_d)^2 n_d^2} \ .\end{aligned} \tag{11}$$

The limit $r=0$ can be taken in (11) and the result for χ at the bulk critical point is, in this Gaussian approximation,

$$\chi_{t=0} = \left(\frac{8}{\pi^2}\right)^d \frac{L^2}{\pi^2} \sum_{\mathbf{n}}{}^{\rm o} \frac{(n_1 n_2 \cdots n_d)^{-2}}{n_1^2 + n_2^2 + \cdots + n_d^2} \ , \tag{12}$$

where we have taken $L_1 = L_2 = \cdots = L_d = L$. The sum in (12) is convergent and can be evaluated numerically in any dimensionality. The values of $\sum_{\mathbf{n}}^{\rm o}$ for $d=5$, 6, 7, and 8 are, respectively, 0.2651(1), 0.2446(1), 0.2344(1), and 0.2312(1). Furthermore, we expect (12) to apply *as an exact leading order result* in more than four dimensions. Thus, we find that χ indeed goes like L^2 at the bulk critical temperature when $d>4$ and free boundary conditions are imposed.

To investigate in more detail the temperature dependence of the susceptibility, we split the region $r \le 0$ into three parts. They are the following: (1) $r_R > 0$ and $r_R = O(L^{-2})$; (2) $|r_R| = O(L^{-d/2})$; (3) $r_R < 0$ and $r_R = O(L^{-2})$. Here

$$r_R \equiv r + (\pi/L_1)^2 + \cdots + (\pi/L_d)^2 \ . \tag{13}$$

Note that the region 2 about $r_R = 0$ is much narrower in the limit of large L than regions 1 and 3 when $d>4$. Before proceeding, note that the mean-field parameter r is just the inverse of the bulk high-temperature susceptiblity. Thus, if

$$\chi(L=\infty, T \to T_c+) \approx Ct^{-1} \ , \tag{14}$$

where C has dimensions of (length)^2, we can define the shifted reduced temperature $\tilde{t}$ corresponding to the shift (13), via

$$\tilde{t} = t + C \sum_{j=1}^{d} (\pi/L_j)^2 \ . \tag{15}$$

We now consider the behavior of the susceptibility of a finite system in the three regions defined above.

Region 1. Here expression (11) yields the leading-order contribution to χ. In this region $\chi \propto L_{\rm min}^2$, where $L_{\rm min}$ is the smallest L_j. The susceptibility is given by (11) in the scaling form

$$\chi \approx L^2 Y(\tilde{t}L^2) \ , \tag{16}$$

which is consistent with the general relation (4). (We omit the explicit dependence on the shape ratios L_i/L_j.) Thus one can set $u=0$ in (4) when $\tilde{t}L^2 = O(1)$.

Region 2. Here the contribution of the lowest-lying standing wave, with all $n_j = 1$, must be evaluated separately. Other modes contribute only corrections to the leading behavior. Since the lowest-lying mode becomes unstable as $r_R \to 0+$ in the harmonic approximation, we retain terms quartic in the amplitude of that mode, which we denote as A_0, in the effective Hamiltonian (9). The contribution of this mode to the susceptibility is

$$\begin{aligned}\chi &= \left(\frac{8}{\pi^2}\right)^d \frac{\int A_0^2 e^{-r_R A_0^2/2 - (3^d u/2^d V) A_0^4} dA_0}{\int e^{-r_R A_0^2/2 - (3^d u/2^d V) A_0^4} dA_0} \\ &= u^{-1/2} L^{d/2} Z(u^{-1/2} \tilde{t} L^{d/2}) \ ,\end{aligned} \tag{17}$$

where the latter scaling form is obtained by a standard change in the integration variable.[2,3,5,6] Note that all the shape dependence here comes through $\tilde{t}$, which is scaled by $L^{d/2} \equiv V^{1/2}$. Inspection of (17) reveals that χ varies significantly in the narrow range of $\tilde{t} = O(L^{-d/2})$. The behavior of the leading order contribution to χ in region 2 is essentially identical to that of systems with periodic boundary conditions in the region $t = O(L^{-d/2})$; see Refs. 3–6 for details. Indeed, by using (17) one can show that

$$\chi_{\text{free}} = \left(\frac{8}{\pi^2}\right)^d \chi_{\text{periodic}}(r \to r_R,\ u \to (\tfrac{3}{2})^d u) \tag{18}$$

in region 2, up to "corrections to scaling."[10] It is also clear that the scaling form of (17) is consistent with (4); however, the uL^{4-d} dependence is singular.

Let us stress that our analysis of the scaling forms appropriate to regions 1 and 2 does not cover the *crossover* between the limiting behaviors. Indeed, on the borderline, anharmonic couplings, e.g., $A_{\mathbf{k}}^2 A_0^2$, etc., become nonnegligible. Thus, one faces an intrinsically multimode ("many-body") problem.[11]

Region 3. Here also the leading order contribution comes entirely from the lowest-lying mode. A complication develops, however. In addition to acquiring a sizable amplitude, the mode starts to distort, developing the spatial dependence of the order-parameter profile in the low-temperature phase that satisfies the appropriate boundary conditions. To properly treat this distortion, it is necessary to abandon the expansion in standing waves and adopt a Ginzburg-Landau-type approach.[12] One solves the mean-field equation

$$-\nabla^2 M(\mathbf{x}) + rM(\mathbf{x}) + 4u[M(\mathbf{x})]^3 = 0 \tag{19}$$

for the order-parameter profile subject to the condition $M(\mathbf{x}) = 0$ on the boundary. A nonzero solution for $M(\mathbf{x})$ will build up in region 3. The leading order contribution to the susceptibility is of $O(L^d)$ and is given by[2]

$$\left[\int_V M(\mathbf{x})\, d^d x\right]^2 / L^d\ . \tag{20}$$

It is known[2] that this *leading* contribution is consistent with the finite-size scaling relation (4). Further progress within the single-mode-type analysis can be achieved by approximating the path integral in (9) by an integration over a family of profiles. The smallest amplitude profiles must be nearly sinusoidal, while the larger amplitude ones must mimic the $\pm M$ solutions of (19). This type of analysis is needed to describe a crossover between regions 2 and 3.

We have thus shown that the susceptibility near the bulk critical point of the finite $d > 4$ Ising model with free boundary conditions is consistent with both the renormalization-group scaling relation (4) and with the upper bound at bulk T_c ($\chi \leq \text{const} \times L^2$). We have indicated how the leading order contribution to χ can be calculated in the immediate vicinity of the bulk critical point.

Our theoretical predictions (12), (15) [with (14)], and (17) may be tested by numerical Monte Carlo calculations which seem feasible[3,4] at least for $d = 5$. One must, however, employ the appropriate susceptibility, defined with respect to the ordering field h, which has coupling of strength unity [see (9)] to the order parameter σ. The order parameter, in turn, is "normalized" by having the coefficient of the gradient term in (9) equal $\frac{1}{2}$. The procedures of deriving the mean-field equations for given lattice models are rather straightforward and well known,[13] so that identification of h should pose no real problem. [Alternatively, one can allow for an additional adjustable parameter, which will enter in relations (12) and (15).]

We believe that the approach outlined above has applications beyond the scope of the investigation reported here. It is now known[5,6] that ϵ expansions can be carried out for finite systems with periodic boundary conditions below the upper marginal dimensionality, given a properly modified version of mean-field theory to expand about. The calculational strategy proposed here ought to extend below four dimensions, yielding one of the key elements needed to investigate finite systems with non-mean-field-like critical behavior subject to the kinds of boundary conditions one expects to find in nature.

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[1]E. Brézin, J. Phys. (Paris) **43**, 15 (1982).

[2]V. Privman and M. E. Fisher, J. Stat. Phys. **33**, 385 (1983).

[3]K. Binder, M. Nauenberg, V. Privman, and A. P. Young, Phys. Rev. B **31**, 1498 (1985).

[4]K. Binder (unpublished).

[5]E. Brézin and J. Zinn-Justin, Nucl. Phys. B (to be published).

[6]J. Rudnick, H. Guo, and D. Jasnow, J. Stat. Phys. (to be published).

[7]M. E. Fisher, in *Critical Phenomena, Proceedings of the International School of Physics "Enrico Fermi," Course LI*, edited by M. S. Green (Academic, New York, 1971).

[8]P. G. Watson, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1973), Vol. 2, and references therein.

[9]M. E. Fisher, in *Renormalization Group in Critical Phenomena and Quantum Field Theory*, proceedings of a conference, edited by J. D. Gunton and M. S. Green (Temple Univ. Press, Philadelphia, 1974).

[10]S. Singh and R. K. Pathria [Can. J. Phys. **63**, 358 (1985)] reported a similar property for the Bose gas with free boundary conditions. A nonscaling shift, larger than the size of the rounding region, was needed for a scaling description, which was otherwise identical to the periodic case.

[11]M. E. Fisher and V. Privman [Phys. Rev. B **32**, 447 (1985)] studied "interference" of two distinct scaling behaviors, for a different problem.

[12]See, e.g., a review by D. E. Sullivan and M. M. Telo de Gama, in *Fluid Interfacial Phenomena*, edited by C. A. Croxton (Wiley, New York, 1985).

[13]Consult, e.g., R. Pandit and M. Wortis, Phys. Rev. B **25**, 3226 (1982).